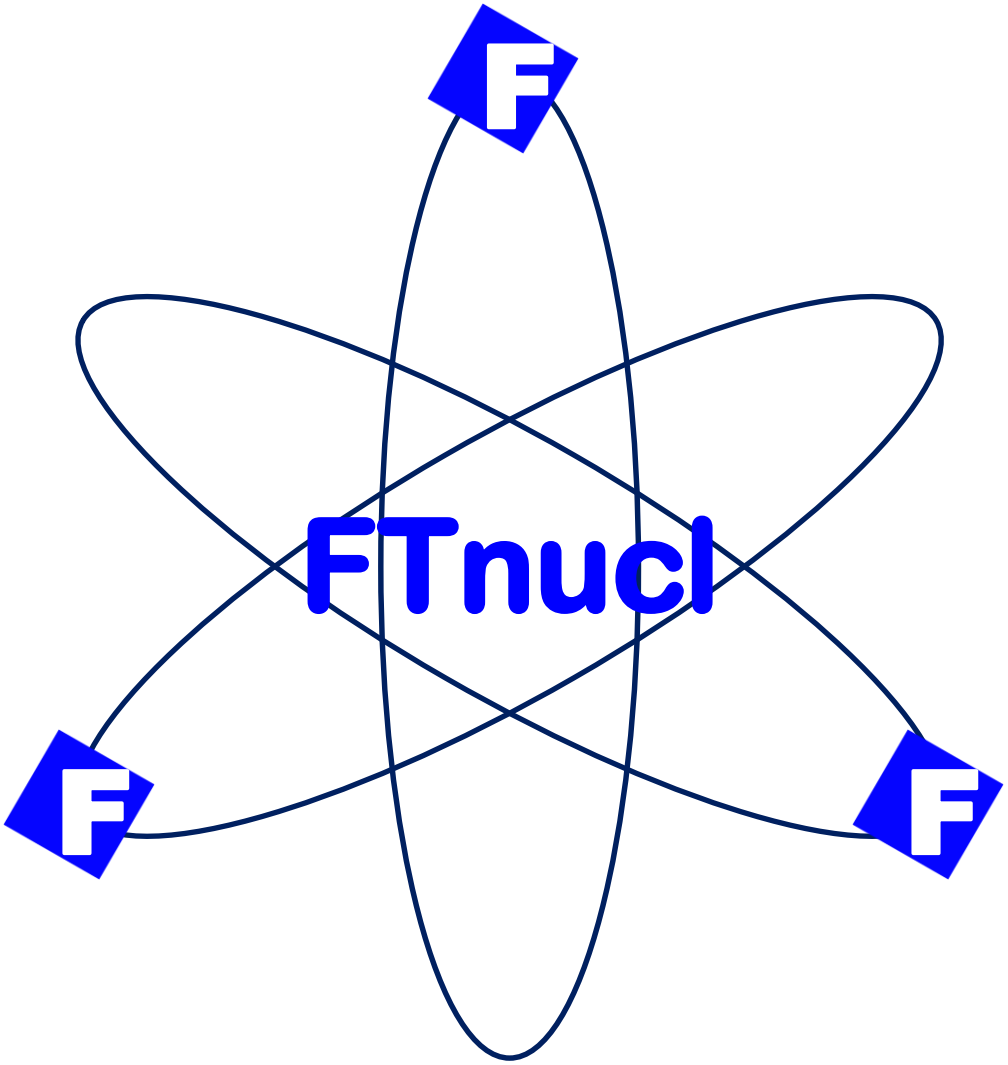


The FACT FTnucl Database

FactSage 7.0

The **FACT FTnucl Database** is a thermochemical database developed for the nuclear industry. It contains thermodynamic data for pure substances and parameters of thermodynamic models for solution phases containing the following elements:

Th, U, Np, Pu, Am

+

Zr, Fe, Ru, Ba

+

Li, Na, K, Rb, Cs

+

C, N, O, I

+

He, Ne, Ar, Kr, Xe, Rn

(note: carbonates, nitrates, nitrites, cyanides, iodates, cyanates and the solubility of noble gases are not included in the molten state)

The **FACT FTnucl Database** can be used for the development of advanced nuclear fuels based on:

- Th, U, Np, Pu and Am
- Oxides
- Carbides, nitrides and carbo-nitrides
- Metals

The **FACT FTnucl Database** can also be used for estimating the thermodynamic behavior and phase relationships involving fission products (based on Cs, I, Zr, Ru, Ba and Rb, and including noble gases Xe, He, Ne, Ar, Kr and Rn) and metallic claddings (Fe, Zr, C).

The **FACT FTnucl Database** must be used with FactSage™ 6.3 or more recent versions, as it fully uses the advantages of the Modified Quasichemical Model in the Quadruplet Approximation (MQMQA) for the liquid metal-oxide-carbide-nitride-iodide solution, which is not implemented in other software.

With FactSage™, materials design is made easier with the use of the **EQUILIB** and **PHASE DIAGRAM Modules** which are based on the well-known **SOLGASMIX Gibbs energy minimizer**:

- Equilibrium, para-equilibrium and constrained equilibrium calculations
- Phase diagrams: T-x_i, T-$P(O_2)$, T-a_C, x_i-$P(O_2)$, isothermal and isoplethal sections, para-equilibrium diagrams, enthalpy diagrams
- Phase transition targets (liquidus, solidus, eutectic, peritectic, boiling points, solvus/solubility limits, etc...)
- Heating curves, boiling points
- Fixed potential calculations

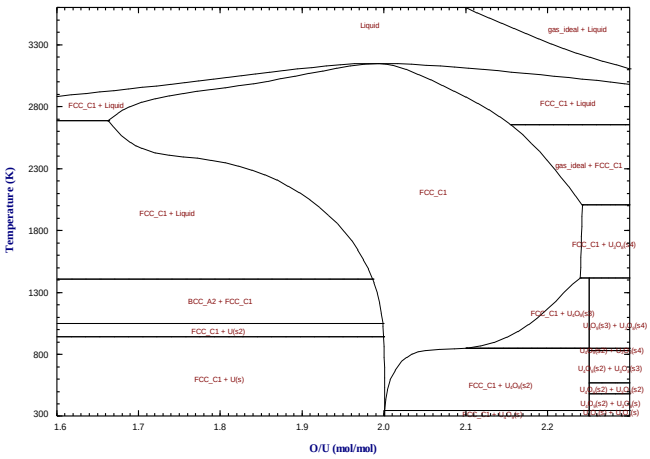
The **FACT FTnucl Database** can benefit from all the capabilities of the software in the field of materials processing:

- High-temperature reaction chemistry: carburizing, nitriding, vapour deposition
- “Open” system calculations
- Stream recycling
- Macro processing
- Amount and composition targets

Some calculated phase diagrams (FTnucl)

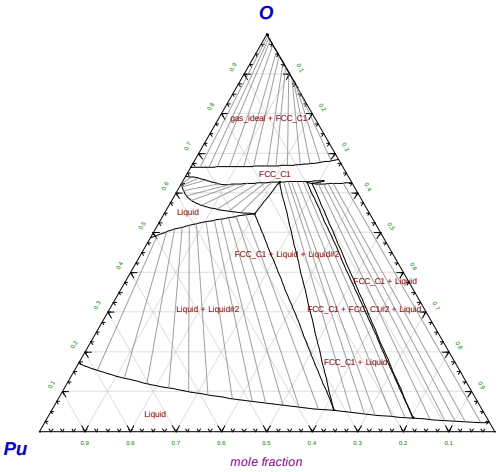
U - O

1 atm

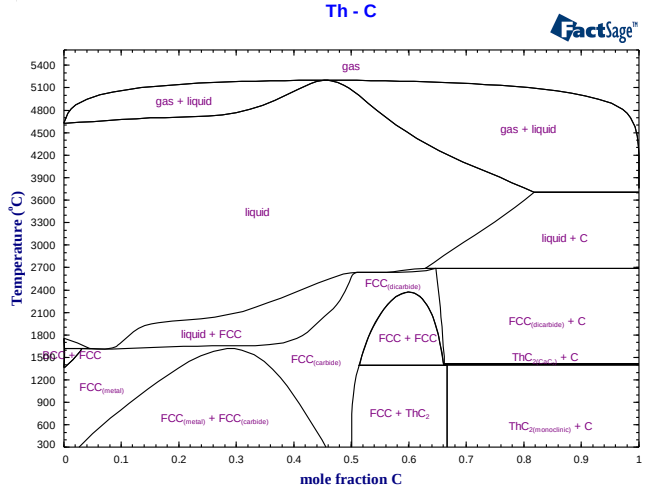


O - U - Pu

2573.15 K, 1 atm



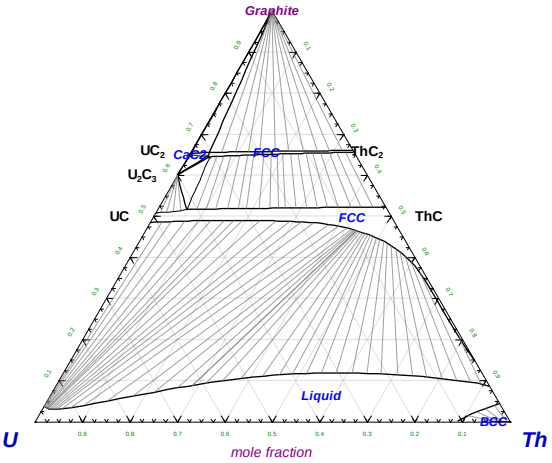
Th - C



1900 K

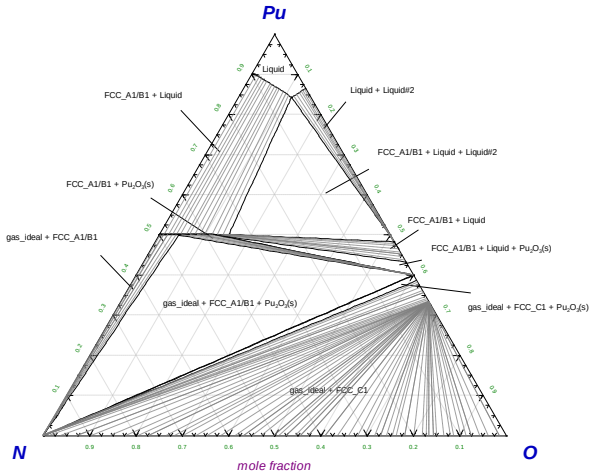
C

Graphite



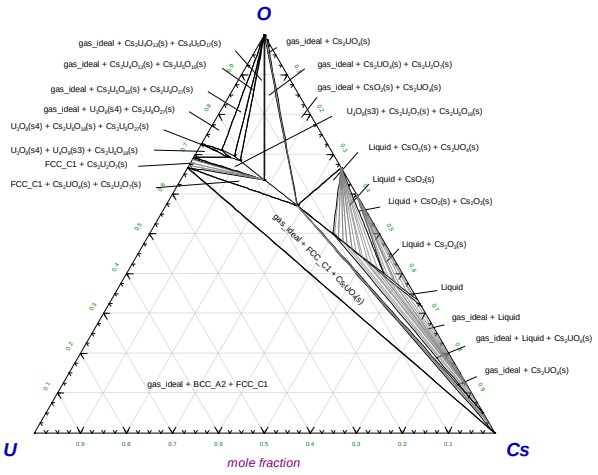
Pu - O - N

2273.15 K, 1 bar



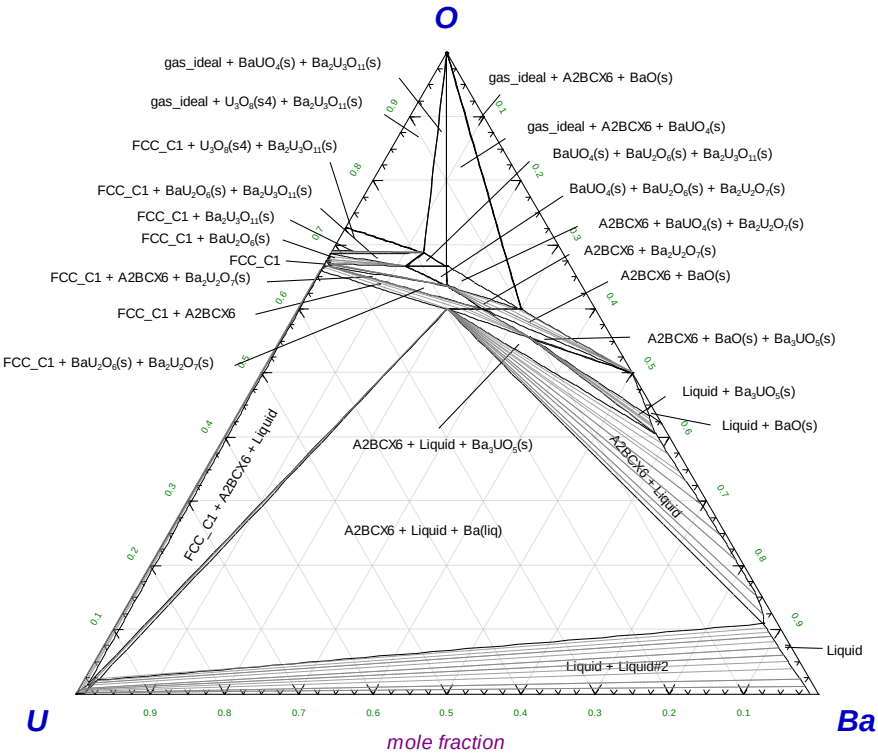
Cs - U - O

1273.15 K, 1 bar



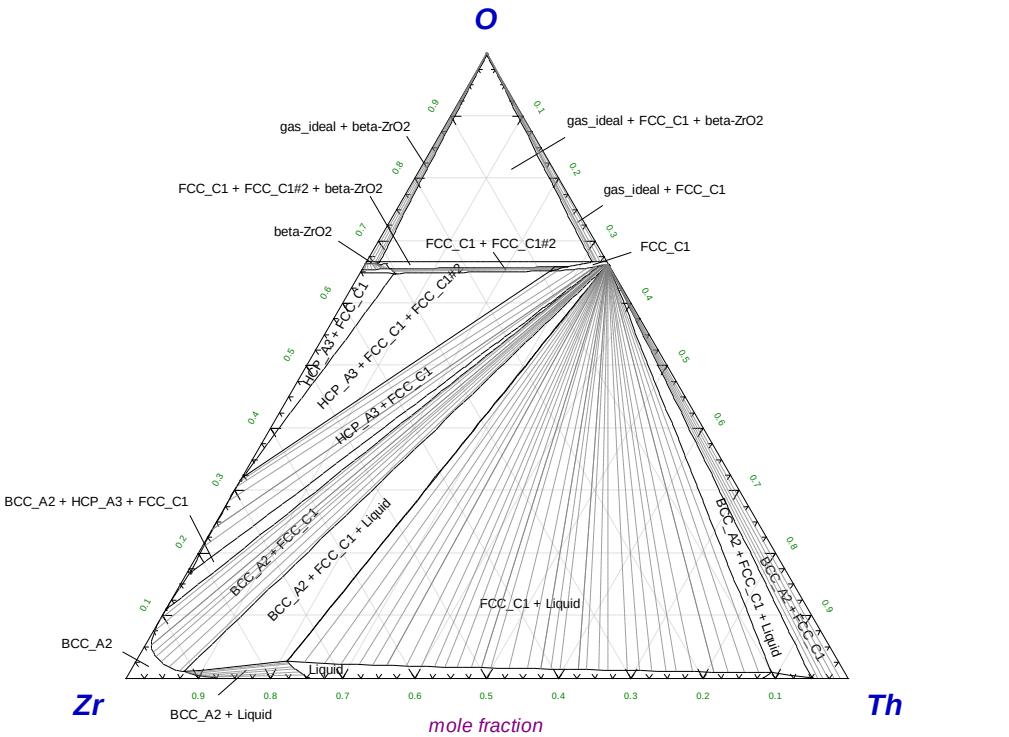
Ba - U - O

1873.15 K, 1 bar



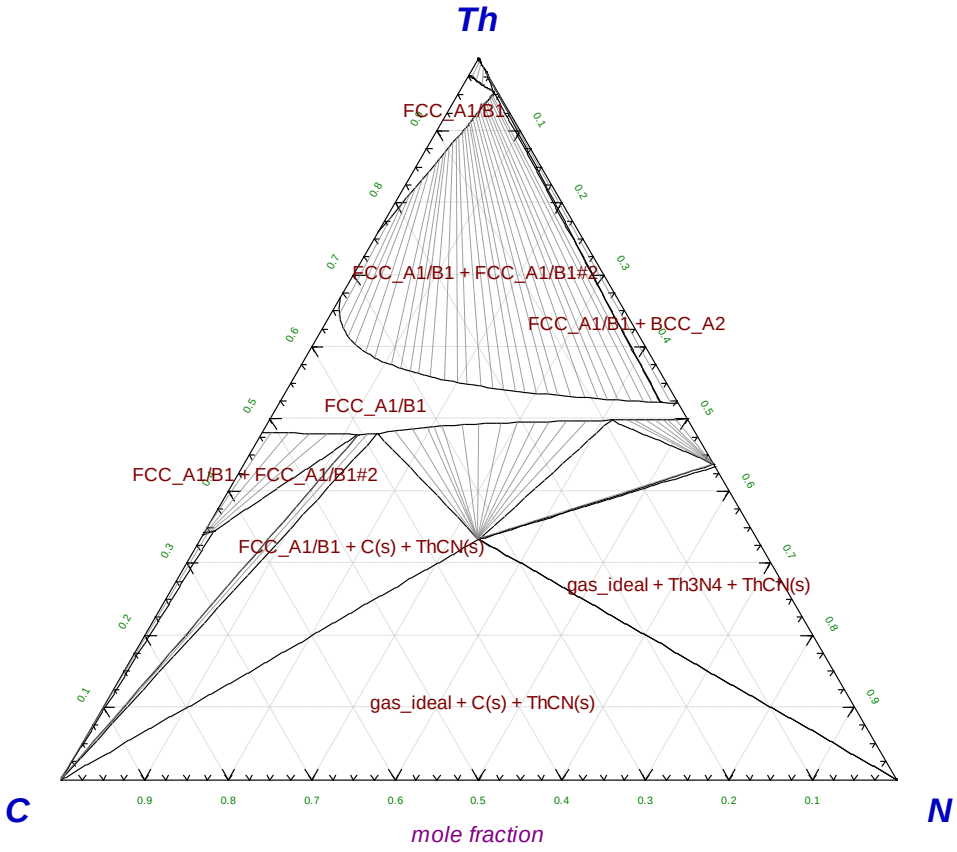
Th - Zr - O

1873.15 K, 1 bar



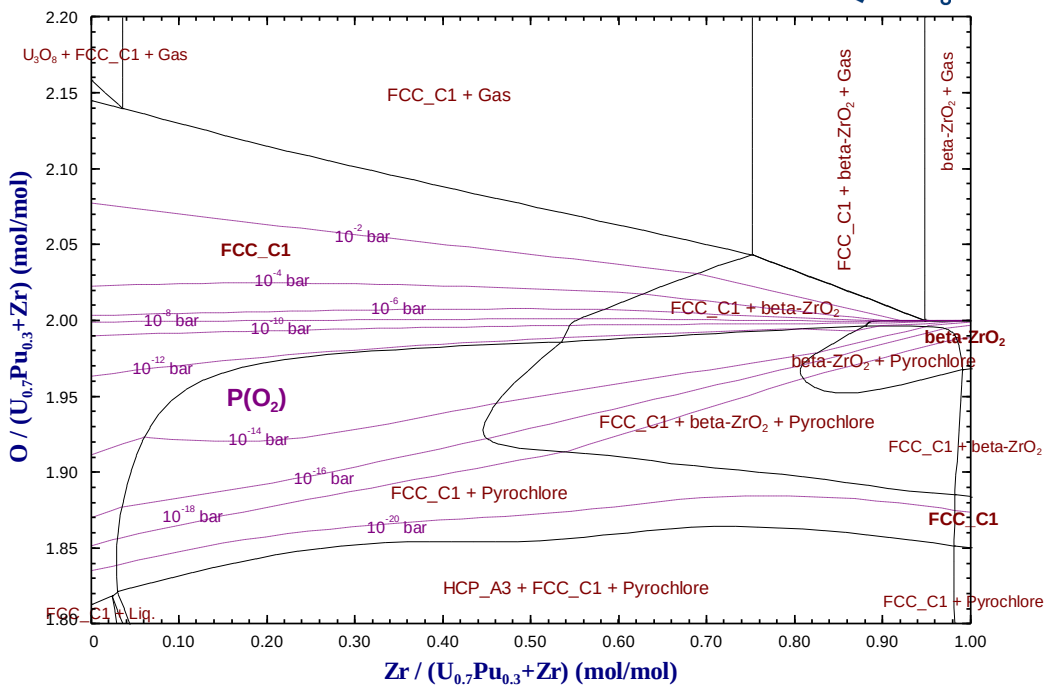
Th - N - C

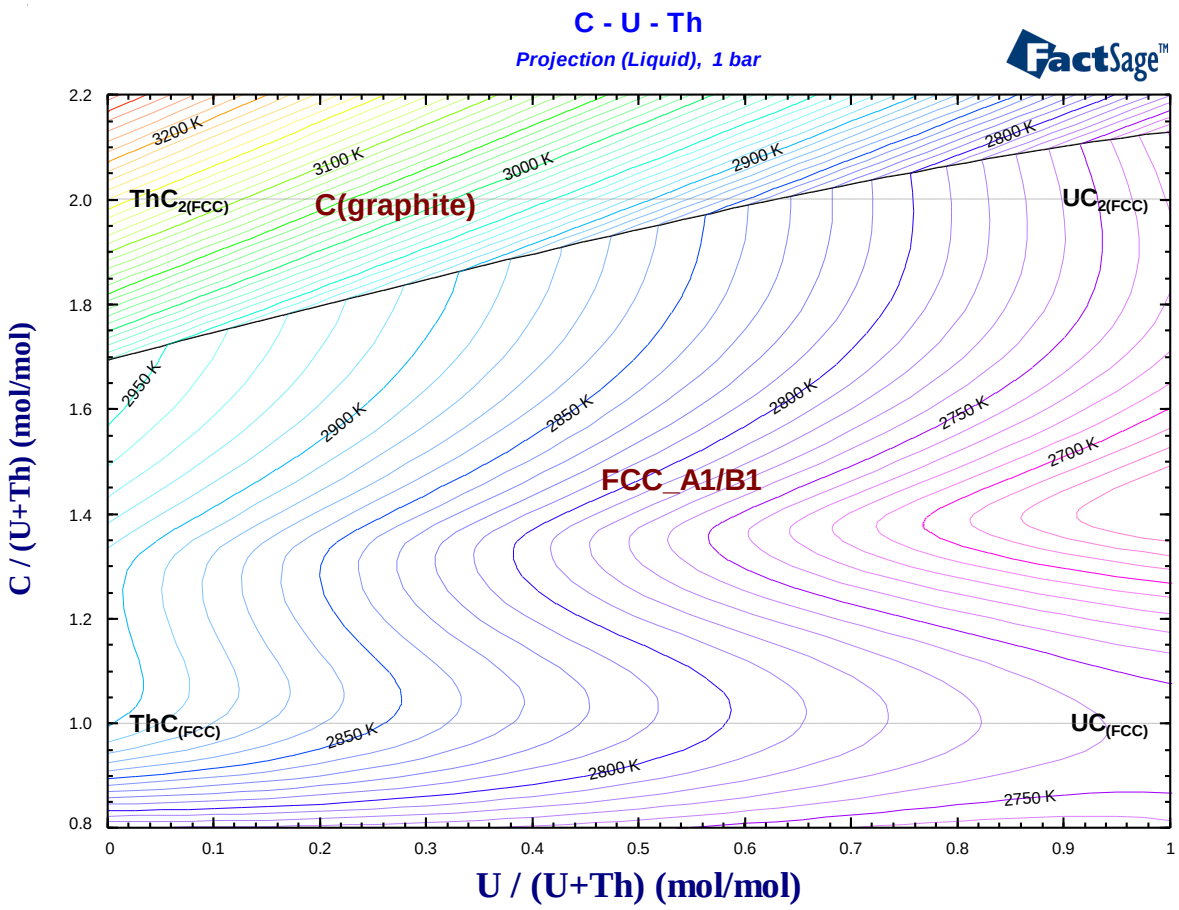
1800 K, 1 atm

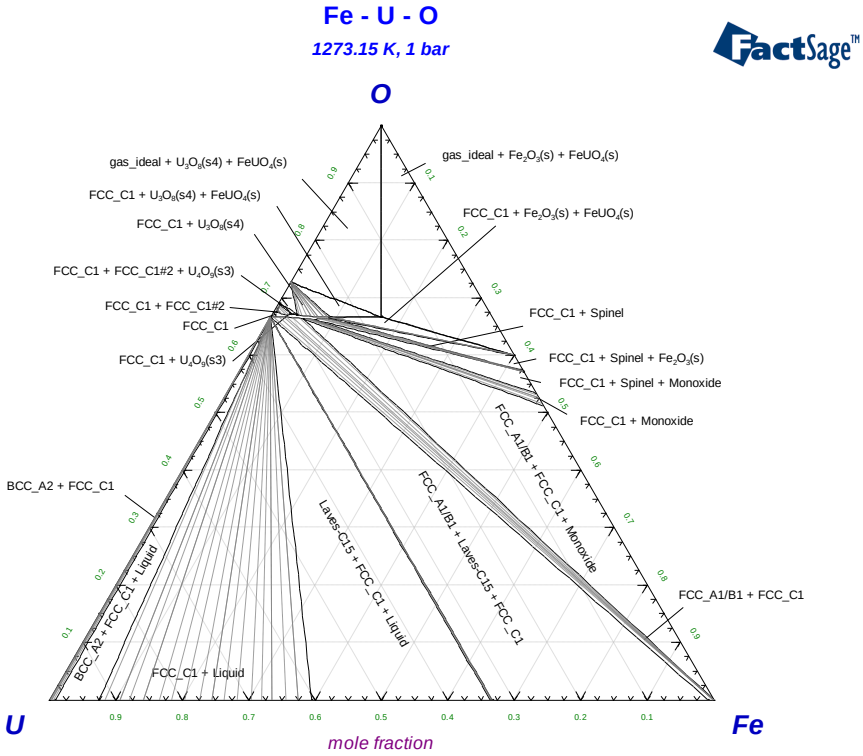


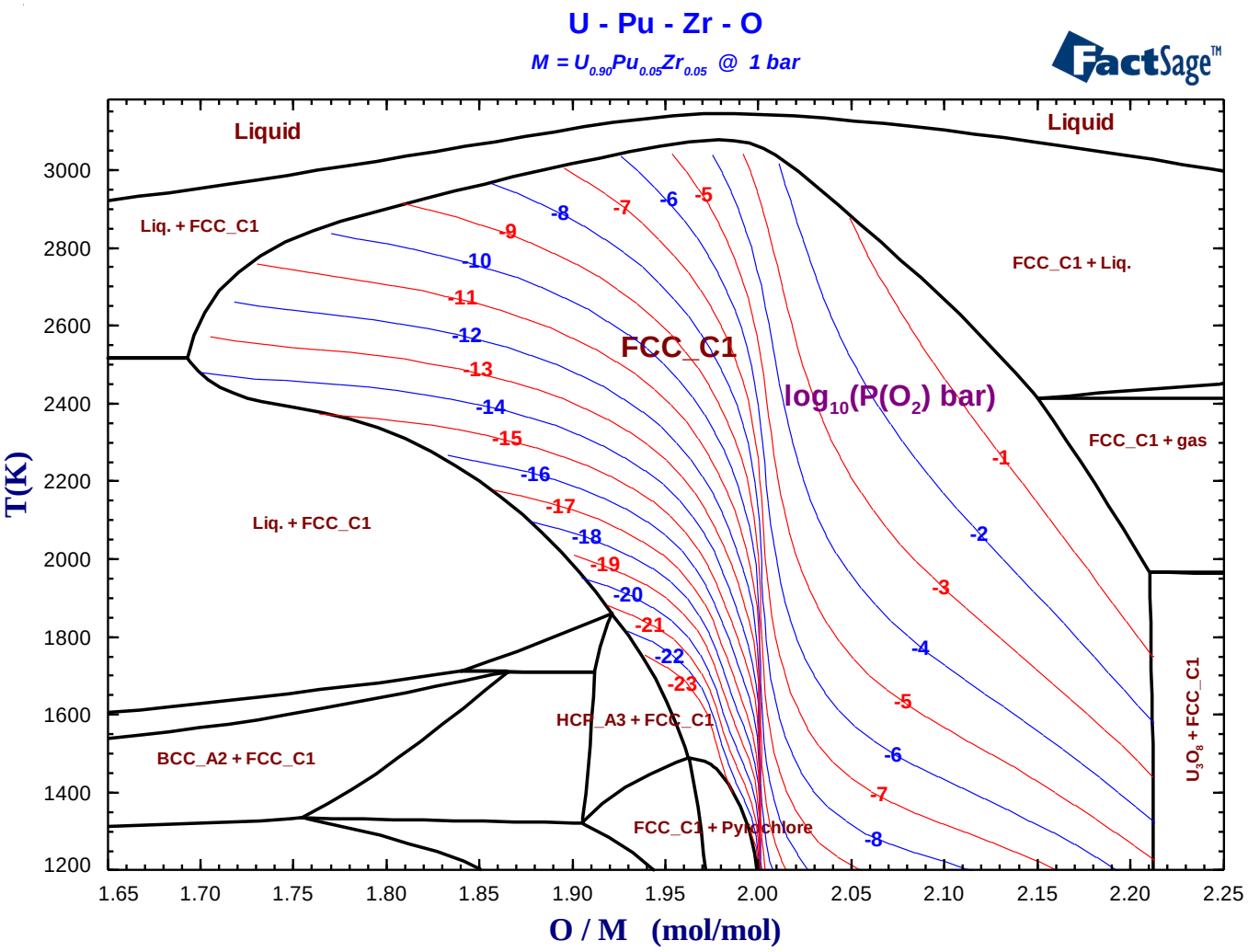
$U_{0.7}Pu_{0.3}$ - Zr - O

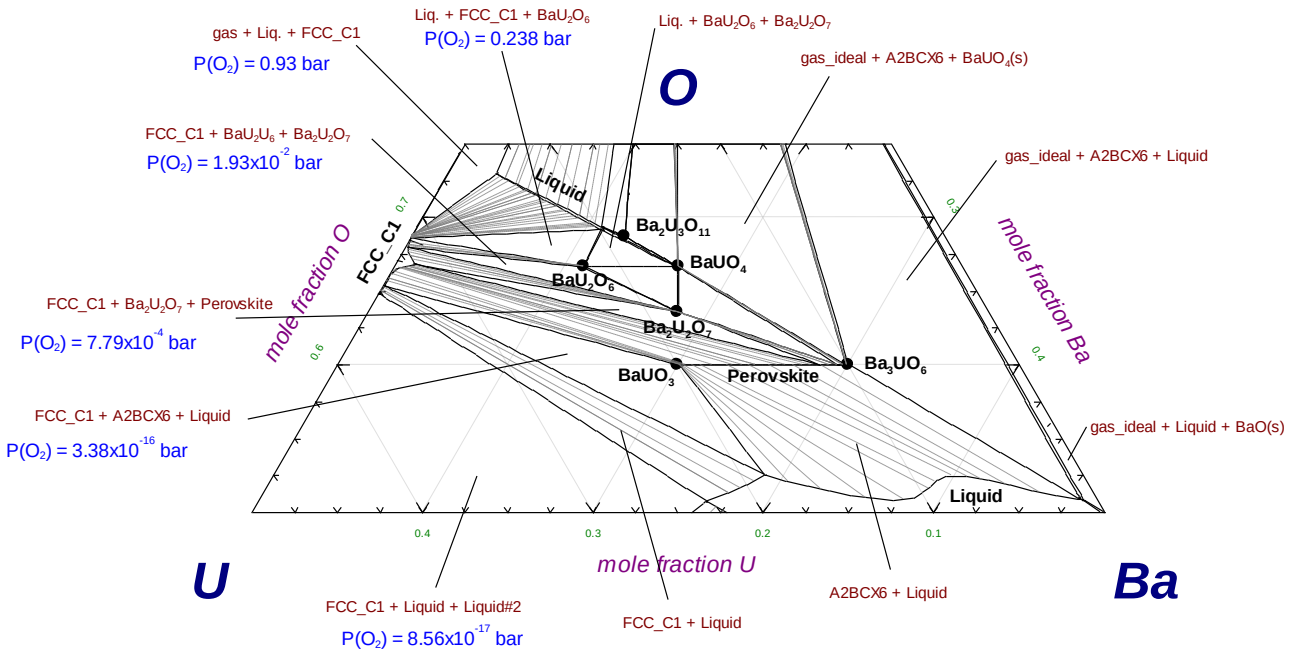
1873.15 K (1 bar)




C - U - Th
Projection (Liquid), 1 bar
FactSage™
ThC2(FCC)
C(graphite)
UC2(FCC)
FCC_A1/B1
ThC(FCC)
UC(FCC)
3200 K
3100 K
3000 K
2900 K
2800 K
2950 K
2900 K
2850 K
2800 K
2750 K
2700 K
2850 K
2800 K
2750 K
C / (U+Th) (mol/mol)
U / (U+Th) (mol/mol)

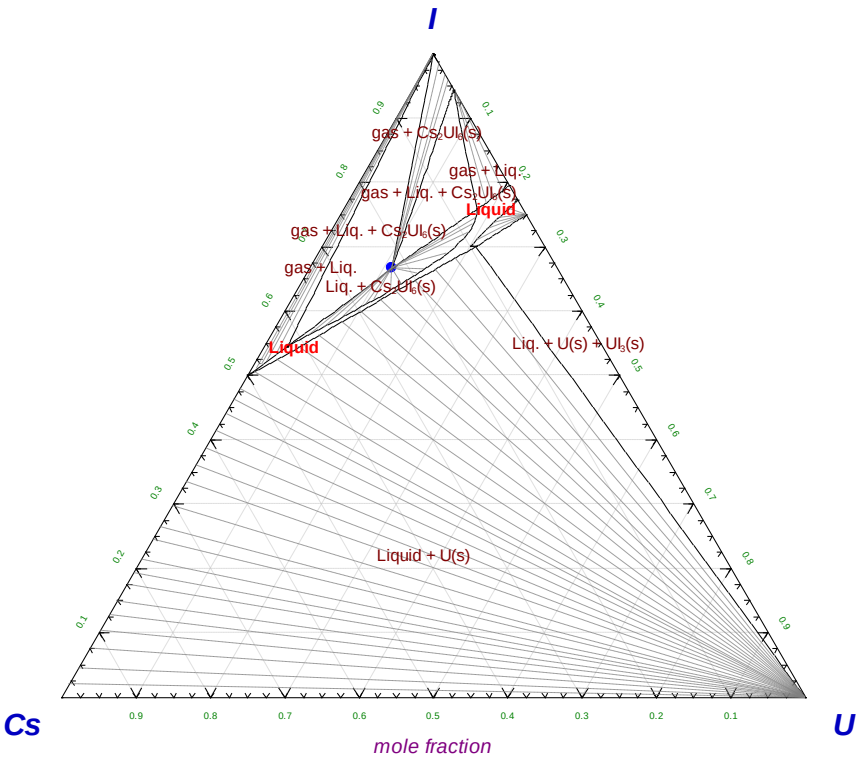

Fe - U - O
1273.15 K, 1 bar
FactSage™
O
U
Fe
mole fraction
gas_ideal + U3O8(s4) + FeUO4(s)
gas_ideal + Fe2O3(s) + FeUO4(s)
FCC_C1 + U3O8(s4) + FeUO4(s)
FCC_C1 + Fe2O3(s) + FeUO4(s)
FCC_C1 + U3O8(s4)
FCC_C1 + FCC_C1#2 + U4O9(s3)
FCC_C1 + Spinel
FCC_C1 + FCC_C1#2
FCC_C1
FCC_C1 + Spinel + Fe2O3(s)
FCC_C1 + U4O9(s3)
FCC_C1 + Spinel + Monoxide
FCC_C1 + Monoxide
FCC_A1/B1 + FCC_C1 + Monoxide
BCC_A2 + FCC_C1
Laves_C15 + FCC_C1 + Liquid
FCC_A1/B1 + Laves_C15 + FCC_C1
FCC_A1/B1 + FCC_C1
BCC_A2 + FCC_C1 + Liquid
FCC_C1 + Liquid


U - Pu - Zr - O
M = U0.90Pu0.05Zr0.05 @ 1 bar
FactSage™
Liquid
Liquid
Liq. + FCC_C1
FCC_C1 + Liq.
FCC_C1
log10(P(O2) bar)
FCC_C1 + gas
Liq. + FCC_C1
HCP_A3 + FCC_C1
BCC_A2 + FCC_C1
FCC_C1 + Pyrochlore
U3O8 + FCC_C1
T(K)
O / M (mol/mol)


gas + Liq. + FCC_C1
P(O2) = 0.93 bar
Liq. + FCC_C1 + BaU2O6
P(O2) = 0.238 bar
Liq. + BaU2O6 + Ba2U2O7
gas_ideal + A2BCX6 + BaUO4(s)
O
FCC_C1 + BaU2O6 + Ba2U2O7
P(O2) = 1.93x10-2 bar
gas_ideal + A2BCX6 + Liquid
Liquid
Ba2U3O11
BaUO4
BaU2O6
FCC_C1
mole fraction O
mole fraction Ba
FCC_C1 + Ba2U2O7 + Perovskite
P(O2) = 7.79x10-4 bar
Ba2U2O7
BaUO3
Perovskite
Ba3UO6
FCC_C1 + A2BCX6 + Liquid
P(O2) = 3.38x10-16 bar
gas_ideal + Liquid + BaO(s)
Liquid
U
mole fraction U
Ba
FCC_C1 + Liquid + Liquid#2
P(O2) = 8.56x10-17 bar
FCC_C1 + Liquid
A2BCX6 + Liquid

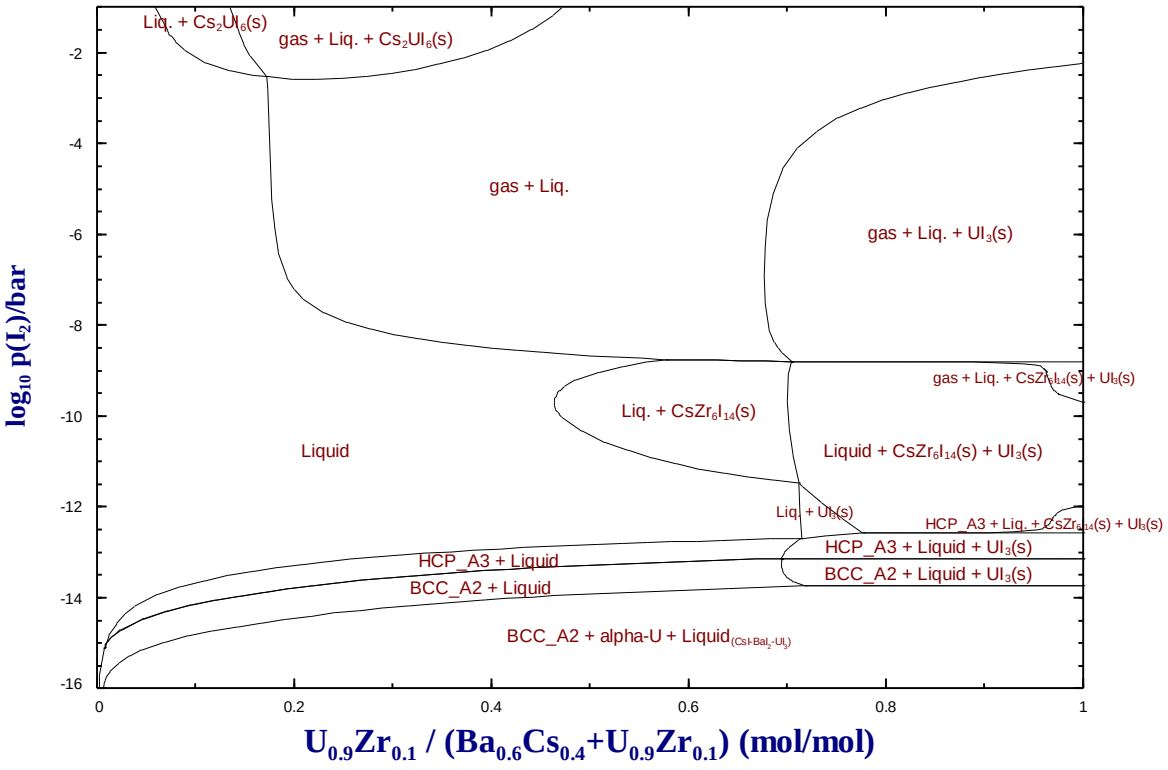
Cs - U - I

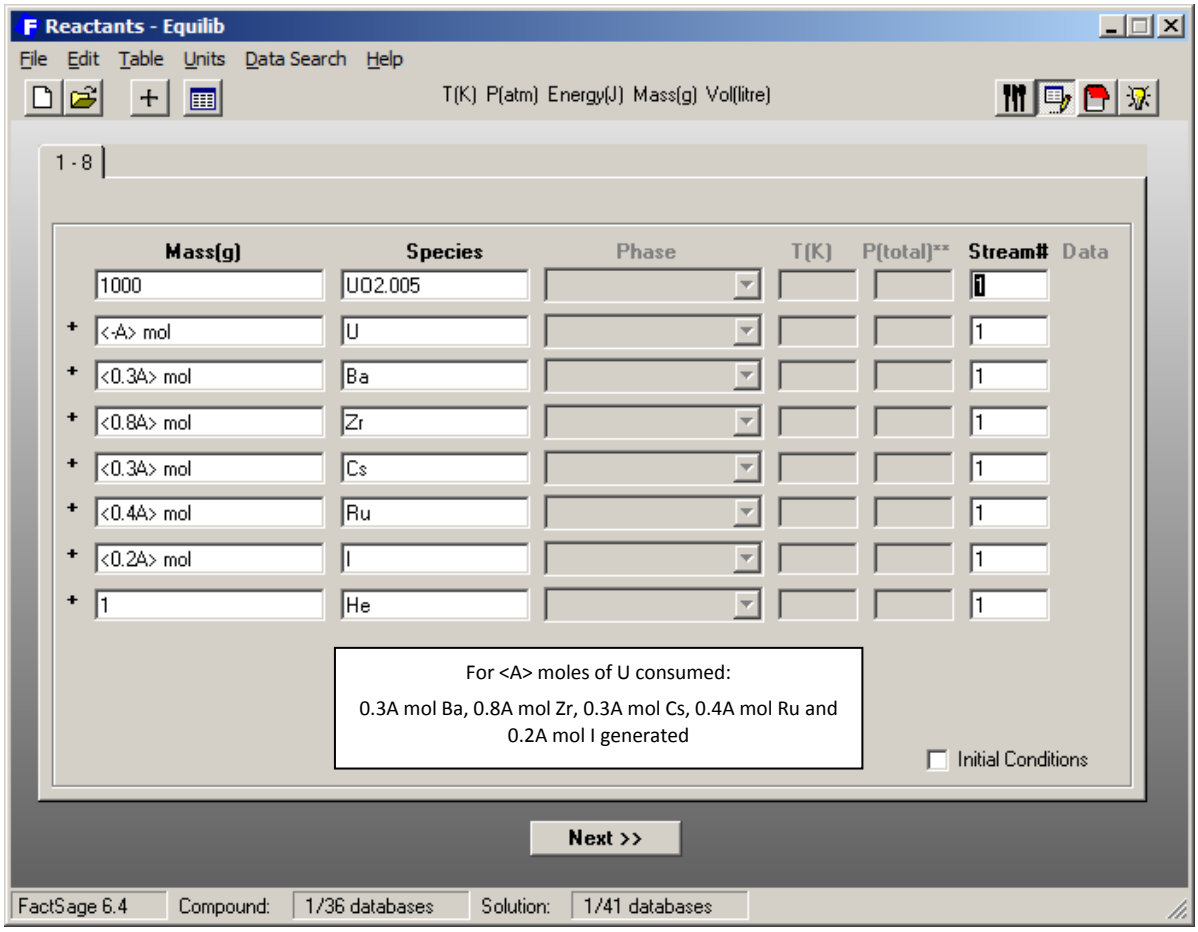
923.15 K, 1 bar

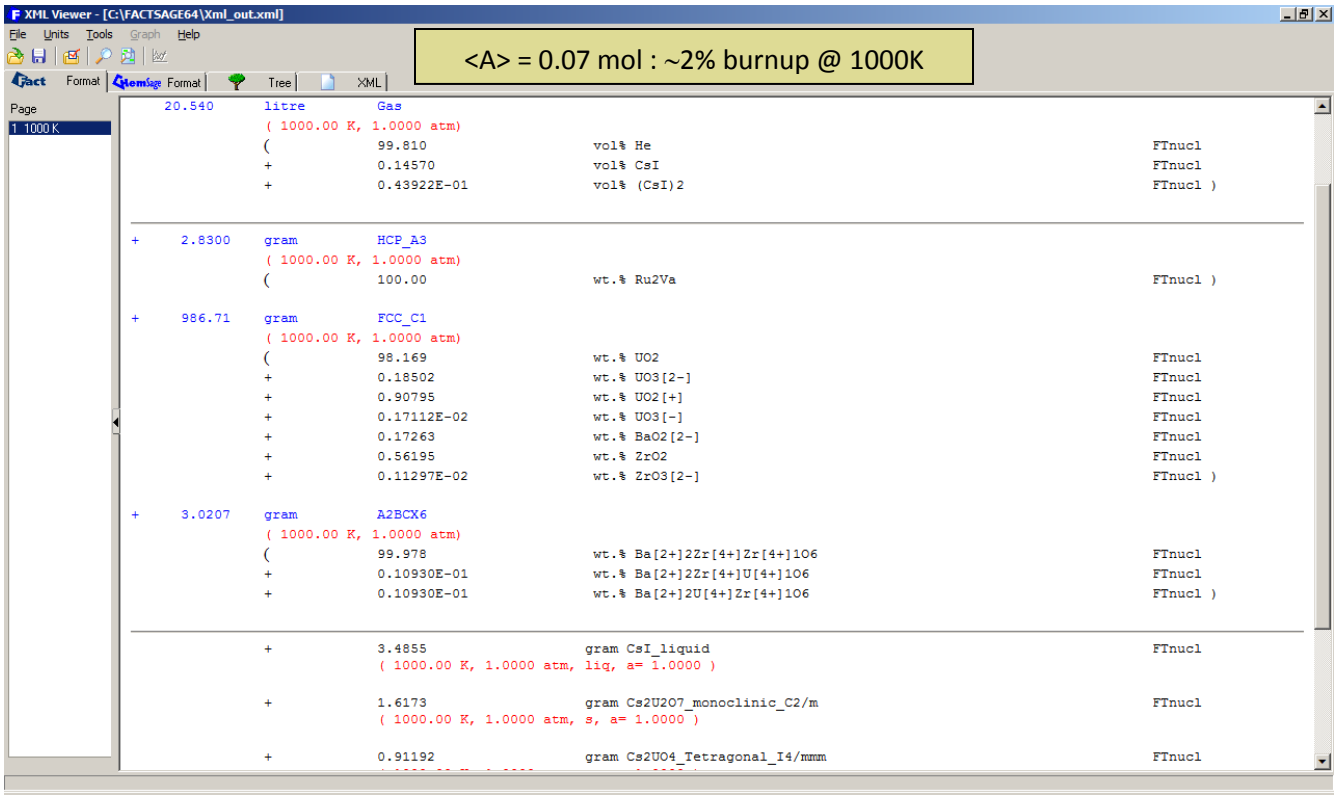


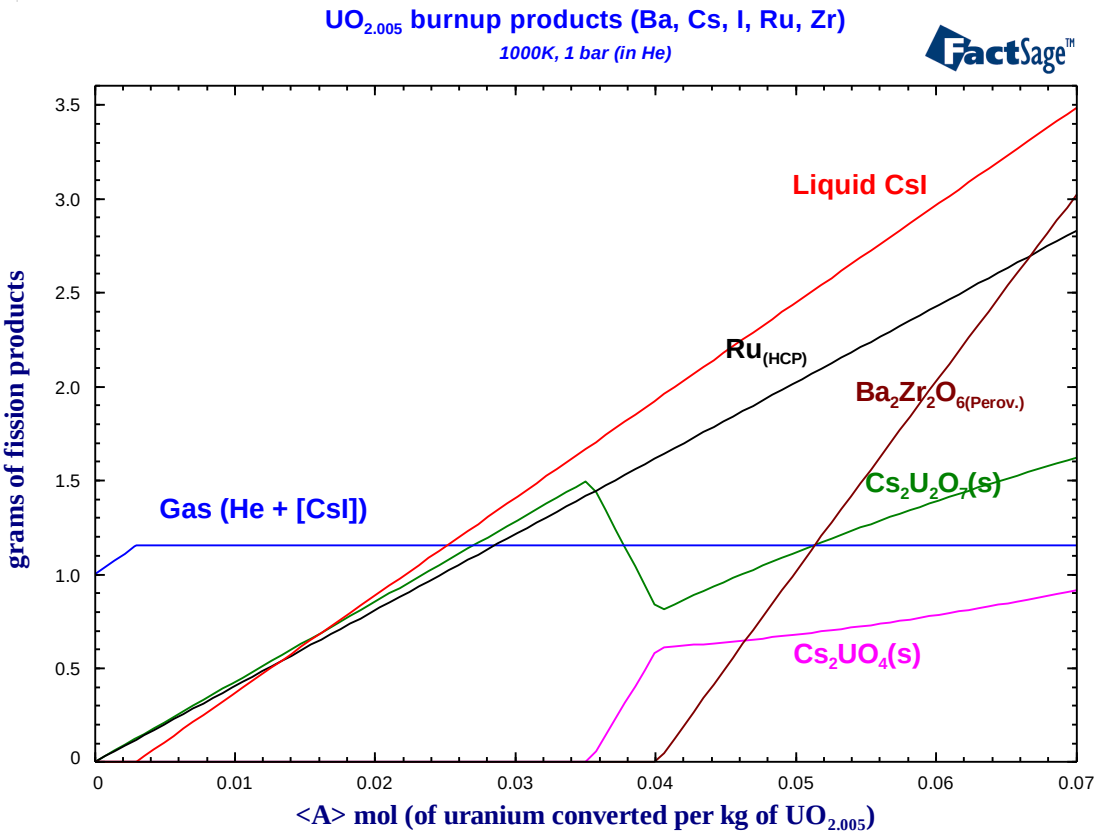
$Ba_{0.6}Cs_{0.4}$ - $U_{0.9}Zr_{0.1}$ - I_2

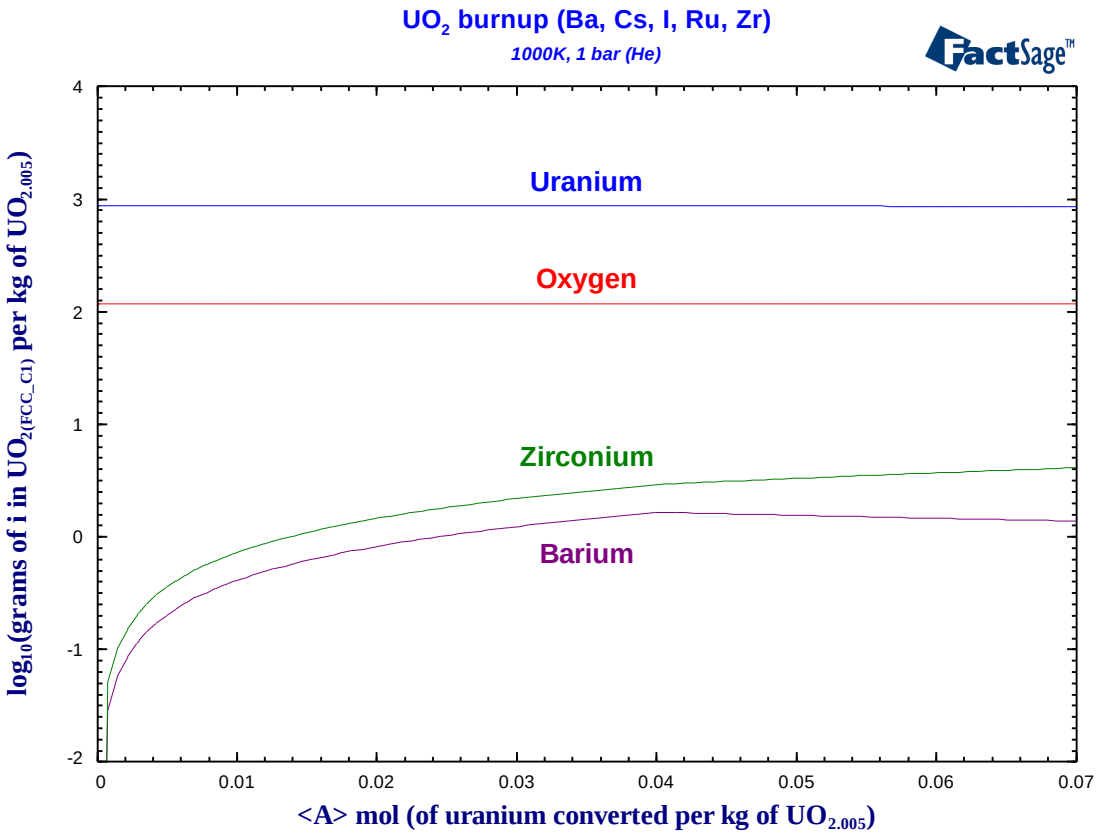
923.15 K, 1 bar




Reactants - Equilib
File Edit Table Units Data Search Help
T(K) P(atm) Energy(J) Mass(g) Vol(litre)
1 - 8
Mass(g) Species Phase T(K) P(total)** Stream# Data
1000 UO2.005 1
<-A> mol U 1
<0.3A> mol Ba 1
<0.8A> mol Zr 1
<0.3A> mol Cs 1
<0.4A> mol Ru 1
<0.2A> mol I 1
1 He 1
For <A> moles of U consumed:
0.3A mol Ba, 0.8A mol Zr, 0.3A mol Cs, 0.4A mol Ru and 0.2A mol I generated
Initial Conditions
Next >>
FactSage 6.4
Compound: 1/36 databases
Solution: 1/41 databases

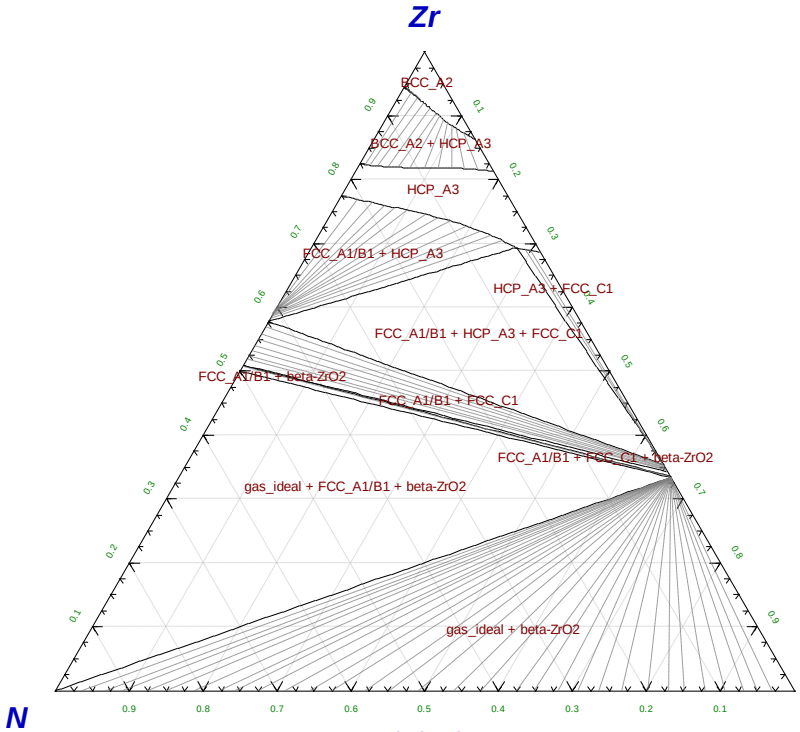

XML Viewer - [C:\FACTSAGE64\Xml_out.xml]
File Units Tools Graph Help
Format Format Tree XML
<A> = 0.07 mol : ~2% burnup @ 1000K
Page
1 1000 K
20.540 litre Gas
(1000.00 K, 1.0000 atm)
(99.810 vol% He FTnucl
+ 0.14570 vol% CsI FTnucl
+ 0.43922E-01 vol% (CsI)2 FTnucl)
+ 2.8300 gram HCP_A3
(1000.00 K, 1.0000 atm)
(100.00 wt.% Ru2Va FTnucl)
+ 986.71 gram FCC_C1
(1000.00 K, 1.0000 atm)
(98.169 wt.% UO2 FTnucl
+ 0.18502 wt.% UO3[2-] FTnucl
+ 0.90795 wt.% UO2[+] FTnucl
+ 0.17112E-02 wt.% UO3[-] FTnucl
+ 0.17263 wt.% BaO2[2-] FTnucl
+ 0.56195 wt.% ZrO2 FTnucl
+ 0.11297E-02 wt.% ZrO3[2-] FTnucl)
+ 3.0207 gram A2BCX6
(1000.00 K, 1.0000 atm)
(99.978 wt.% Ba[2+]2Zr[4+]Zr[4+]1O6 FTnucl
+ 0.10930E-01 wt.% Ba[2+]2Zr[4+]U[4+]1O6 FTnucl
+ 0.10930E-01 wt.% Ba[2+]2U[4+]Zr[4+]1O6 FTnucl)
+ 3.4855 gram CsI_liquid FTnucl
(1000.00 K, 1.0000 atm, liq, a= 1.0000)
+ 1.6173 gram Cs2U2O7_monoclinic_C2/m FTnucl
(1000.00 K, 1.0000 atm, s, a= 1.0000)
+ 0.91192 gram Cs2UO4_Tetragonal_I4/mmm FTnucl


UO2.005 burnup products (Ba, Cs, I, Ru, Zr)
1000K, 1 bar (in He)
FactSage
grams of fission products
<A> mol (of uranium converted per kg of UO2.005)
Liquid CsI
Ru(HCP)
Ba2Zr2O6(Perov.)
Cs2U2O7(s)
Gas (He + [CsI])
Cs2UO4(s)
0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0.01
0.02
0.03
0.04
0.05
0.06
0.07


UO2 burnup (Ba, Cs, I, Ru, Zr)
1000K, 1 bar (He)
FactSage
log10(grams of i in UO2(FCC_C1) per kg of UO2.005)
<A> mol (of uranium converted per kg of UO2.005)
Uranium
Oxygen
Zirconium
Barium
-2
-1
0
1
2
3
4
0.01
0.02
0.03
0.04
0.05
0.06
0.07

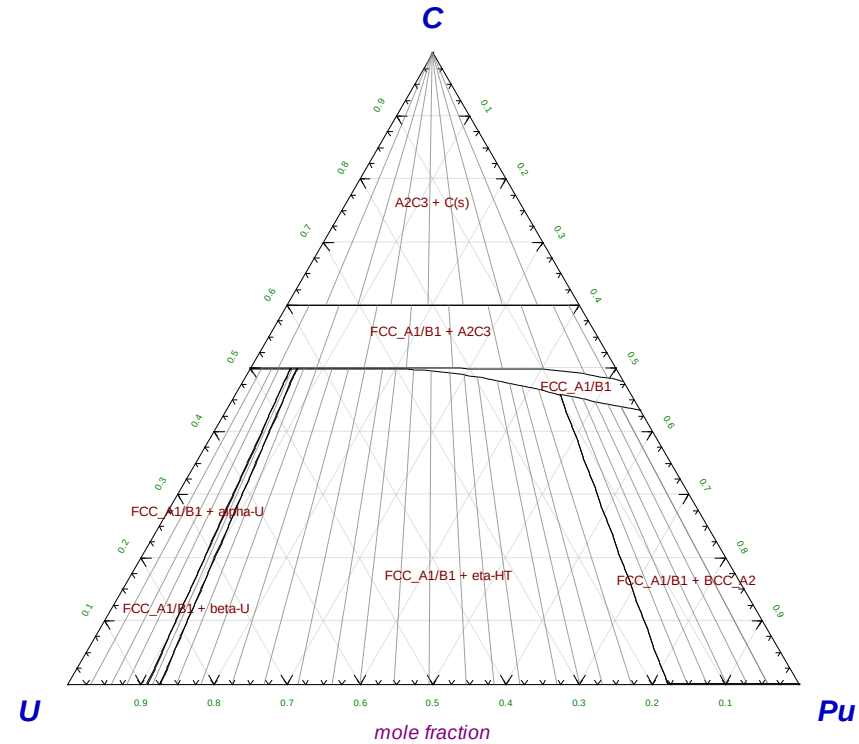
Zr - O - N

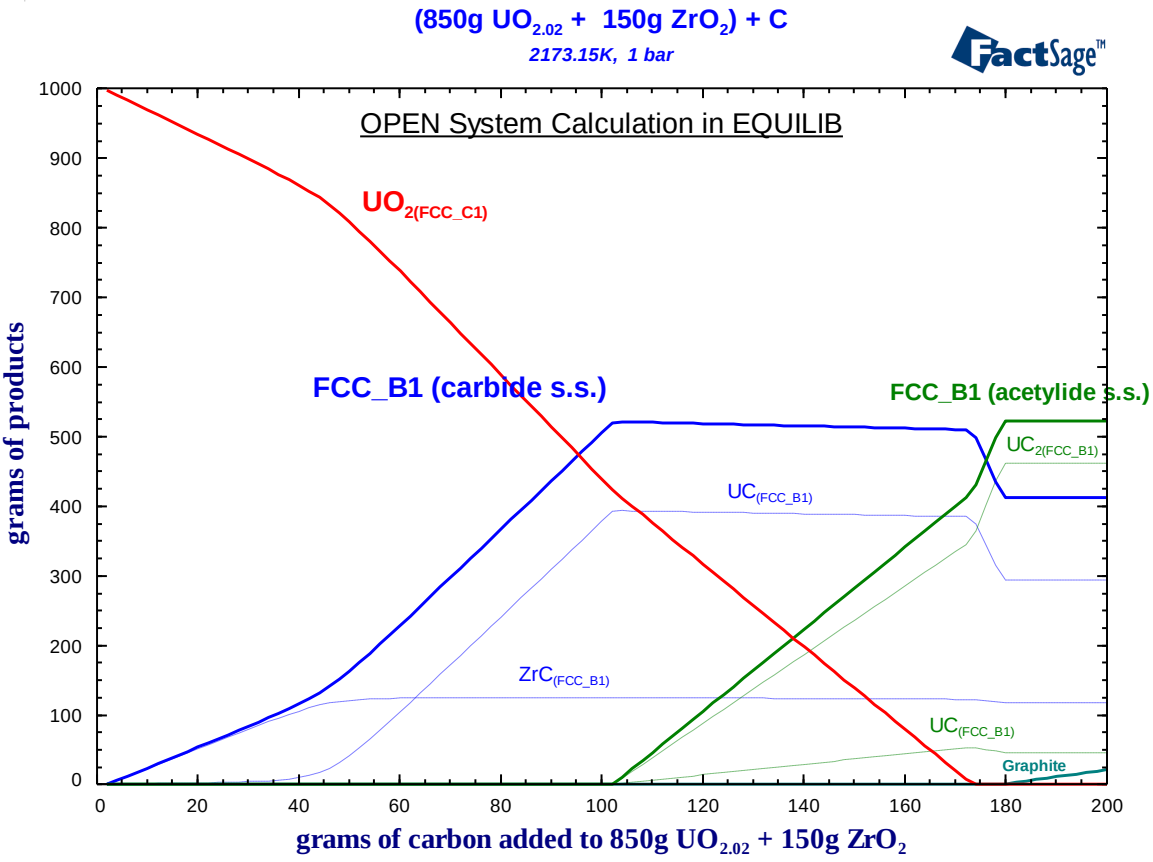
2073.15 K, 1 bar

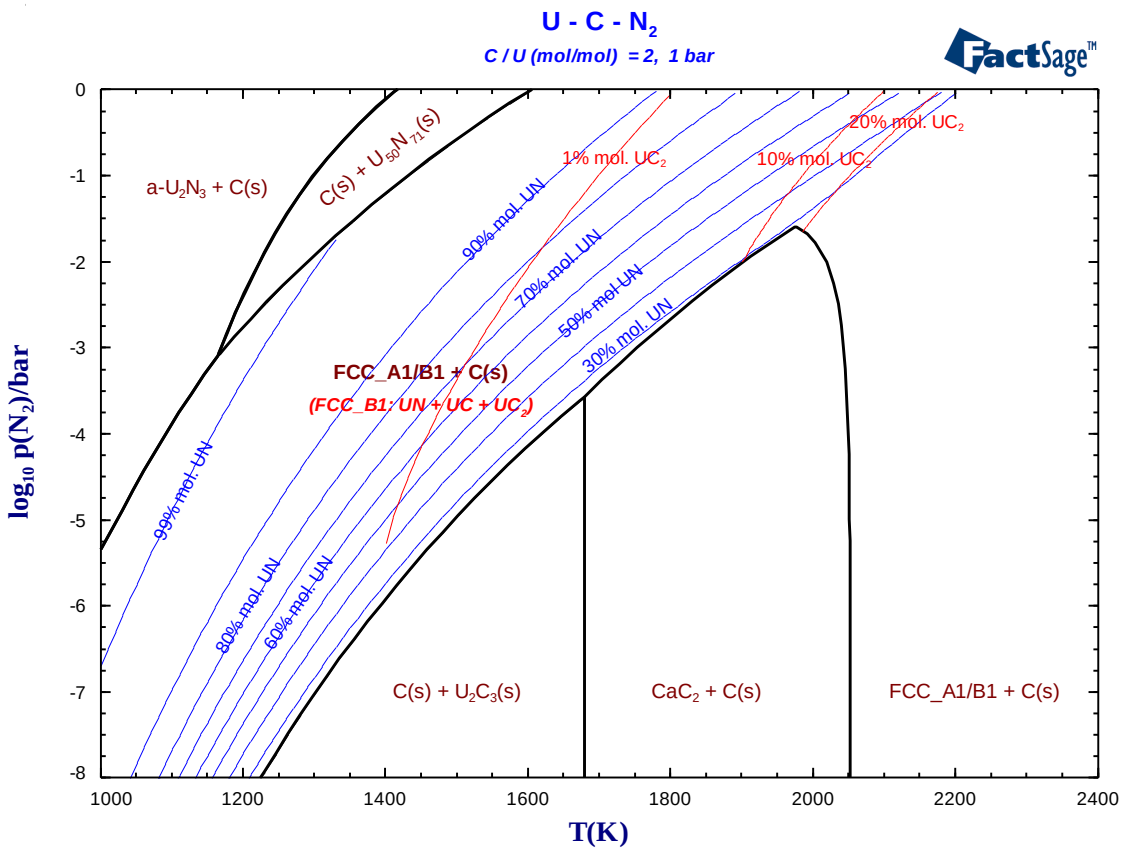


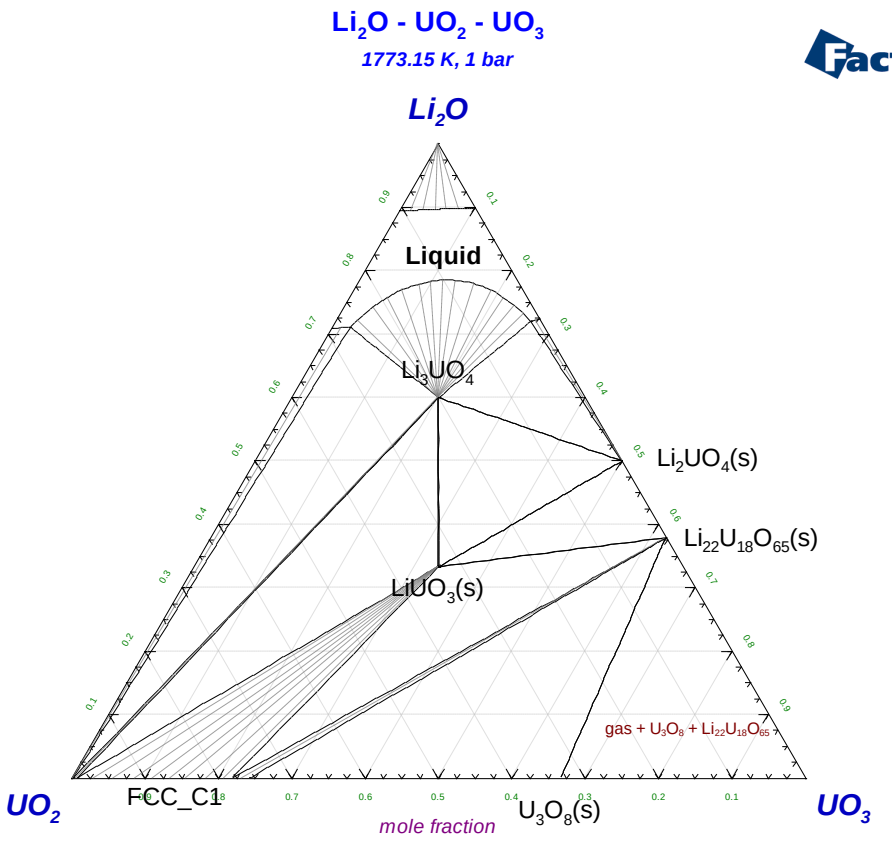
C - Pu - U - paraequilibrium diffusing elements: C

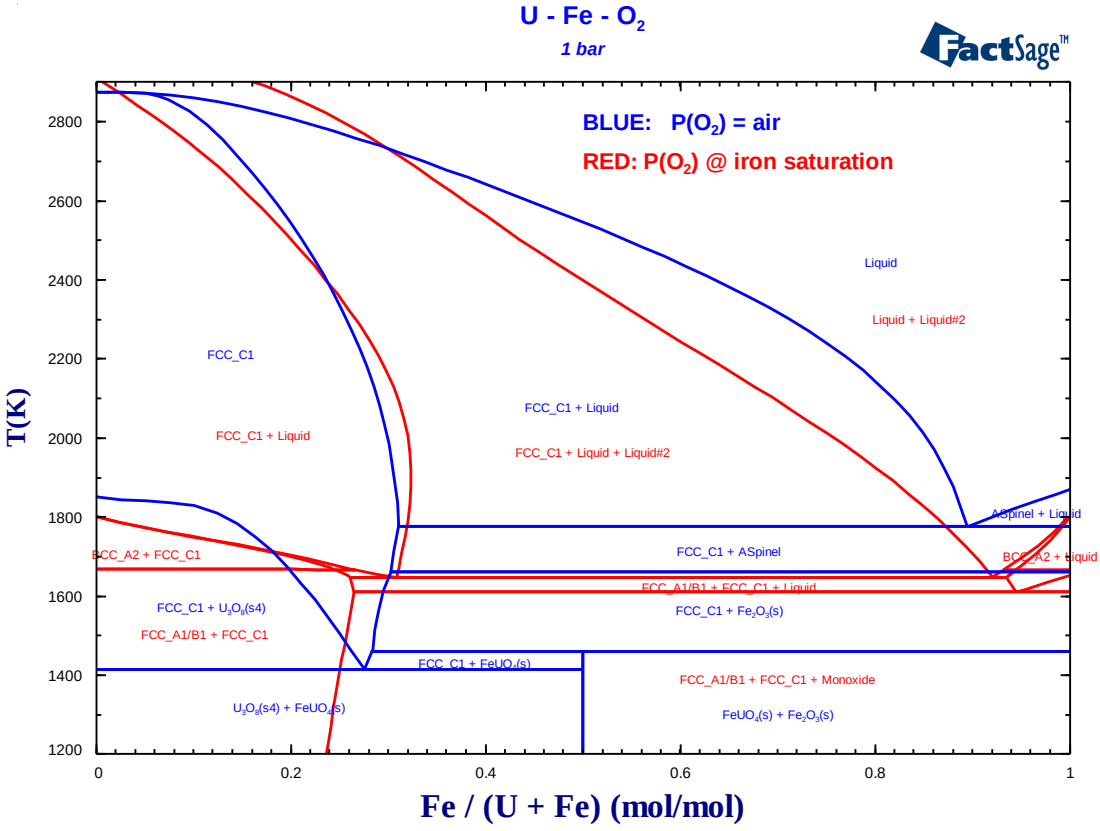
873.15 K, 1 bar




(850g UO2.02 + 150g ZrO2) + C
2173.15K, 1 bar
FactSage
OPEN System Calculation in EQUILIB
UO2(FCC_C1)
FCC_B1 (carbide s.s.)
FCC_B1 (acetylide s.s.)
UC2(FCC_B1)
UC(FCC_B1)
ZrC(FCC_B1)
UC(FCC_B1)
Graphite
grams of products
grams of carbon added to 850g UO2.02 + 150g ZrO2
0
100
200
300
400
500
600
700
800
900
1000
0
20
40
60
80
100
120
140
160
180
200

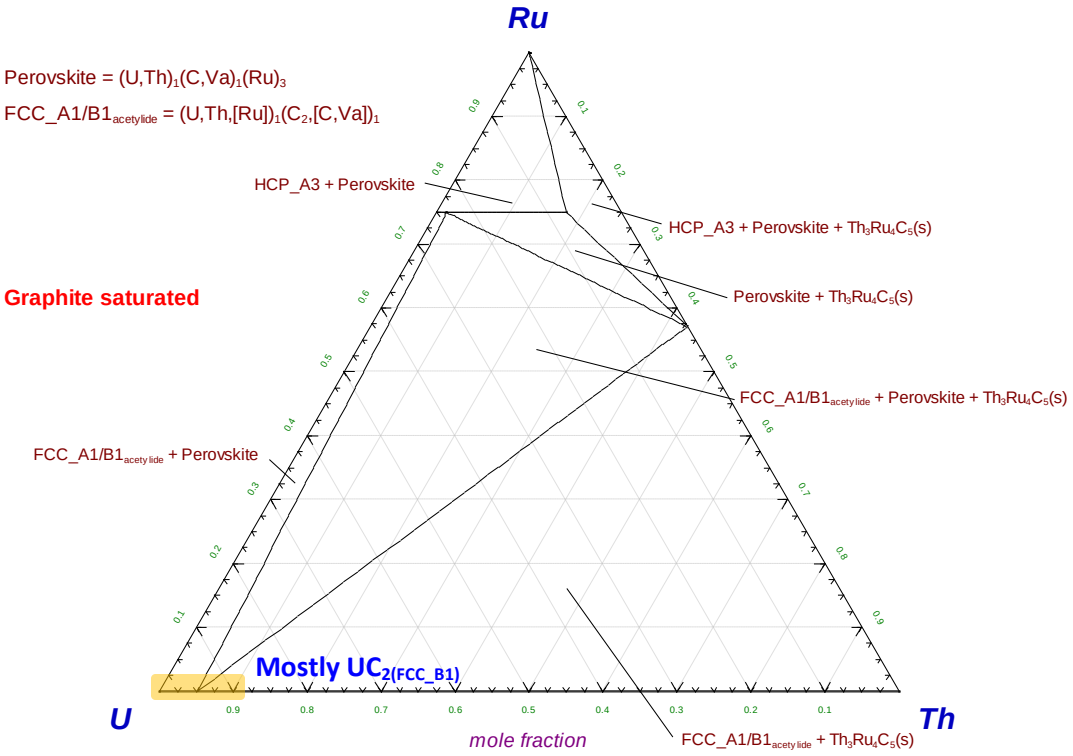

U - C - N2
C / U (mol/mol) = 2, 1 bar
FactSage
a-U2N3 + C(s)
C(s) + U50N71(s)
1% mol. UC2
10% mol. UC2
20% mol. UC2
90%-mol.-UN
70%-mol.-UN
50%-mol.-UN
30%-mol.-UN
99%-mol.-UN
80%-mol.-UN
60%-mol.-UN
FCC_A1/B1 + C(s)
(FCC_B1: UN + UC + UC2)
C(s) + U2C3(s)
CaC2 + C(s)
FCC_A1/B1 + C(s)
log10 p(N2)/bar
T(K)
0
-1
-2
-3
-4
-5
-6
-7
-8
1000
1200
1400
1600
1800
2000
2200
2400


Li2O - UO2 - UO3
1773.15 K, 1 bar
FactSage™
Li2O
Liquid
Li3UO4
Li2UO4(s)
Li22U18O65(s)
LiUO3(s)
gas + U3O8 + Li22U18O65
UO2
FCC_C1
U3O8(s)
UO3
mole fraction


U - Fe - O2
1 bar
FactSage™
BLUE: P(O2) = air
RED: P(O2) @ iron saturation
Liquid
Liquid + Liquid#2
FCC_C1
FCC_C1 + Liquid
FCC_C1 + Liquid + Liquid#2
ASpinel + Liquid
FCC_A2 + FCC_C1
FCC_C1 + ASpinel
FCC_A2 + Liquid
FCC_A1/B1 + FCC_C1 + Liquid
FCC_C1 + U3O8(s4)
FCC_C1 + Fe2O3(s)
FCC_A1/B1 + FCC_C1
FCC_C1 + FeUO4(s)
FCC_A1/B1 + FCC_C1 + Monoxide
U3O8(s4) + FeUO4(s)
FeUO4(s) + Fe2O3(s)
T(K)
Fe / (U + Fe) (mol/mol)

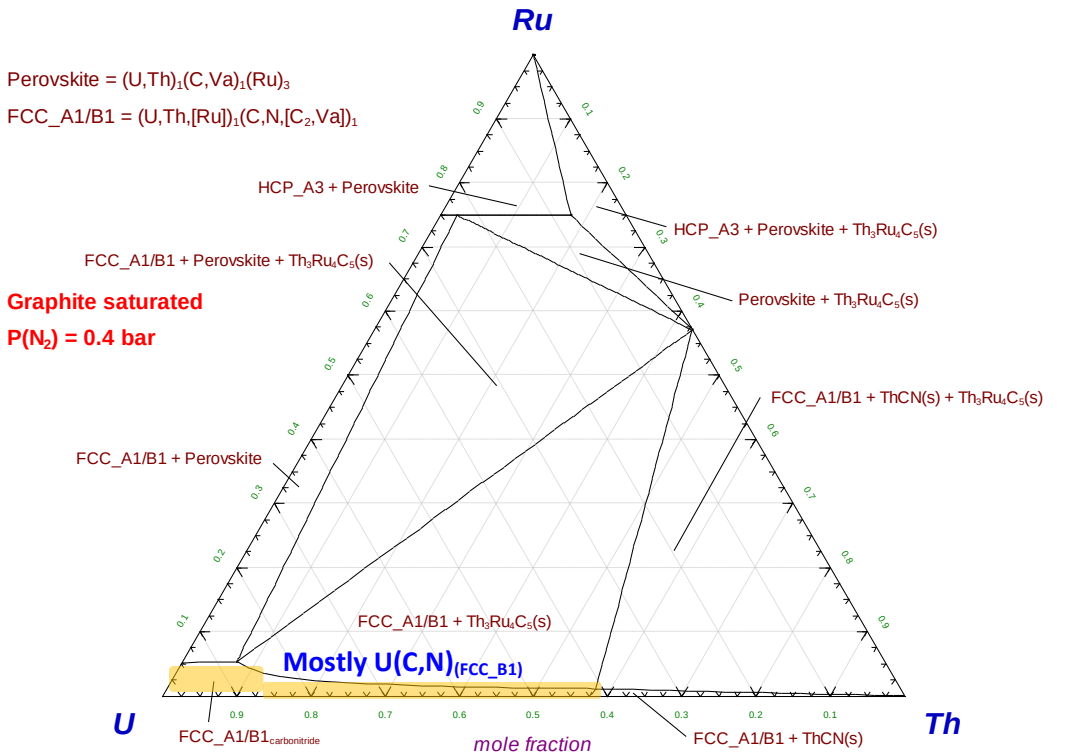
U - Th - Ru - C

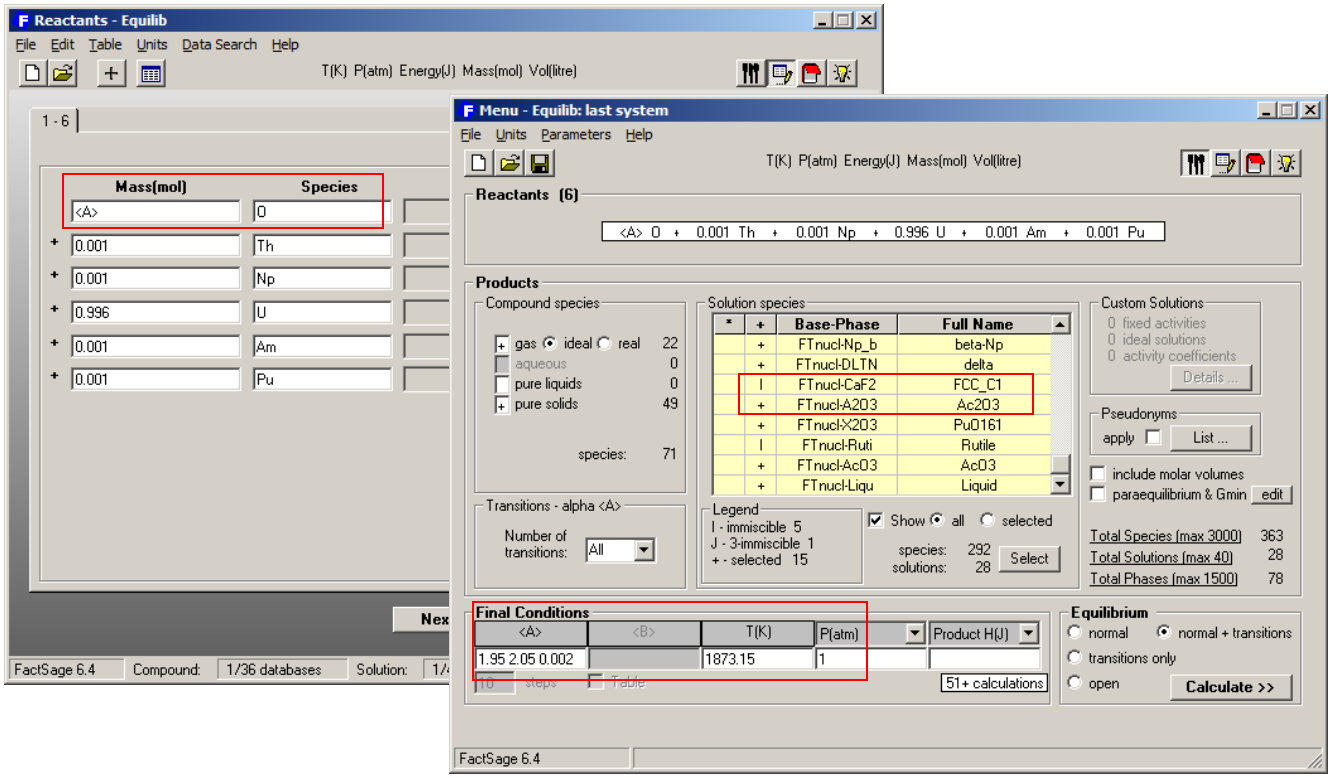
a(C(s)) = 1, 2073.15 K, 1 bar



U - Th - Ru - C - N_2

a(C(s)) = 1, P(N_2) = 0.4 bar, 2073.15 K, 1 bar





0.996 U + 0.001 Th + 0.001 Np + 0.001 Am + 0.001 Pu (mol)

1873.15K, 1 bar